Hydro motion in WDM*

J. J. Barnard[1], R. M. More[2], J. Armijo[2] A. Zylstra[2]

Warm Dense Matter School

10-16 January, 2008

Berkeley, California, USA

1. LLNL 2. LBNL

*This work was performed under the auspices of the U.S. Department of Energy by LLNL under contract DE-AC52-07NA27344, the University of California, LBNL under Contract Number DE-AC02-05CH1123.

Outline of talk

1. Motivation for understanding hydrodynamic motion in WDM

2. Euler Equations, EOS and Volumetric energy deposition

3. Theory and simulations of planar targets
   - -- Solid foils
   - -- Exploration of two-phase regime
     - Existence of temperature/density "plateau"
     - Maxwell construction
   - -- Parameter studies of more realistic targets
   - -- Foam slabs
   - -- Droplets and bubbles

Understanding hydrodynamics is needed to help determine EOS

One of the goals of WDM research is to determine the Equation of State (i.e. the generalized relation between Pressure P, Density ρ and Temperature T) for materials with high vaporization temperatures. More generally, the relationship between entropy s, energy density ε, mean ionization state Z^*, as well P, ρ and T is desired.

Ideally, instantaneous volumetric energy deposition (with a known energy deposition rate) and direct measurement of T allows a determination of ε, ρ, and T. However, for instantaneous heating to be obtained hydrodynamic motion must be negligible.

When hydrodynamic motion is observed, the motion is driven by pressure gradients, so that the pressure is observed indirectly, in principle yielding information about the EOS.

The "Euler equations" describe fluid motion

Mass conservation:
$$\frac{\partial \rho}{\partial t} = -\nabla \cdot (\rho v)$$

Acceleration:
$$\rho \frac{\partial v}{\partial t} = -\rho v \cdot \nabla v - \nabla p$$

Change of energy per gram:
$$d\varepsilon = T ds + \frac{p}{\rho^2} d\rho$$

(First and second laws of thermodynamics)

Entropy equation:
$$\frac{\partial s}{\partial t} = -v \cdot \nabla s \quad + \quad \dot{s}_{source}$$

Energy equation (consequence of previous 4 equations)
$$\frac{\partial}{\partial t}\left(\rho\varepsilon + \frac{1}{2}\rho v^2\right) = -\nabla \cdot \left(\left[\varepsilon + \frac{v^2}{2} + \frac{p}{\rho} \right] \rho v \right) + \rho \dot{\varepsilon}_{source}$$

The equations may be written in Lagrangian form

Convective derivative: $$\frac{d}{dt} = \frac{\partial}{\partial t} + v \cdot \nabla$$

Mass conservation equation: $$\frac{d\rho}{dt} = -\rho \; \nabla \cdot v$$

Acceleration equation $$\rho \frac{dv}{dt} = - \; \nabla p$$

Adiabatic flow condition: $$\rho \frac{ds}{dt} = \rho \dot{s}_{source}$$

In Lagrangian form, the energy conservation equation reads:

$$\frac{d}{dt}\left(\rho\varepsilon + \frac{1}{2}\rho v^2\right) = -\nabla \cdot (pv) - \left(\rho\varepsilon + \frac{1}{2}\rho v^2\right) \nabla \cdot v \;+\; \rho\dot{\varepsilon}_{source}$$

To close the equations and connect the pressure to the density and temperature an equation of state must be specified

Example EOS's:

Perfect gas: $p = (Z^* + 1)\,\rho\ kT/(Am_{\mathrm{amu}})$

$$\varepsilon = (Z^* + 1)\,kT/\,((\gamma\text{-}1)Am_{\mathrm{amu}})$$

$$s = (Z^* + 1)\,k\ \ln[\varepsilon^{1/(\gamma-1)}/\rho]/(Am_{\mathrm{amu}})$$

$$\Longrightarrow p/p_0 = (\rho/\rho_0)^{\gamma} \text{ for } s = \text{constant}$$

(Here γ= ratio of specific heats = 5/3 for monatonic gas, so $1/(\gamma\text{-}1) = 3/2$)

Van der Waal's fluid:

$$p = \frac{\rho kT}{Am_{amu}(1-b\rho)} - a\rho^2 \qquad \varepsilon = \frac{3kT}{2Am_{amu}} - a\rho$$

$$s = \frac{k}{Am_{amu}}\ln\left(Am_{amu}\frac{(1-b\rho)}{\rho\lambda^3}\right) \quad \textbf{where} \quad \lambda = \sqrt{\frac{h^2}{2\pi Am_{amu}kT}}$$

(a and b are parameters that can be adjusted to match known physicall data such as vaporization point or critical point).

Example EOS's continued:

Zeldovich-Raizer model:

$$p = (Z^* + 1)\,\rho\, kT/(Am_{\mathrm{amu}})$$

$$\varepsilon = 3(Z^* + 1)\, kT/\,(2Am_{\mathrm{amu}}) + Q(Z^*)/(Am_{\mathrm{amu}})$$

$$Q(Z^*) = \sum_{i=1}^{Z^*} I_i$$

$$\frac{N_e N^{i+1}}{N^i} = \frac{g_{i+1}}{g_i}\frac{2(2\pi m_e kT)^{3/2}}{h^3}\exp\left[\frac{-I_{i+1}}{kT}\right]$$

(Calculate Z* approximately by solving non-linear Saha equation)

Thomas-Fermi model:

Calculates electron pressure and mean ion ionization state assuming Fermi-Dirac distribution of electrons in self-consistent electrostatic potential of ion and electrons

QEOS:

Uses Thomas-Fermi model for electron pressure, lattice vibrations for ions (phonons) in solid phase, semi-empirical fluid for ion liquid

SESAME:

Tabulated EOS based on empirical scaling of experimental results

Energy deposition must also be specified

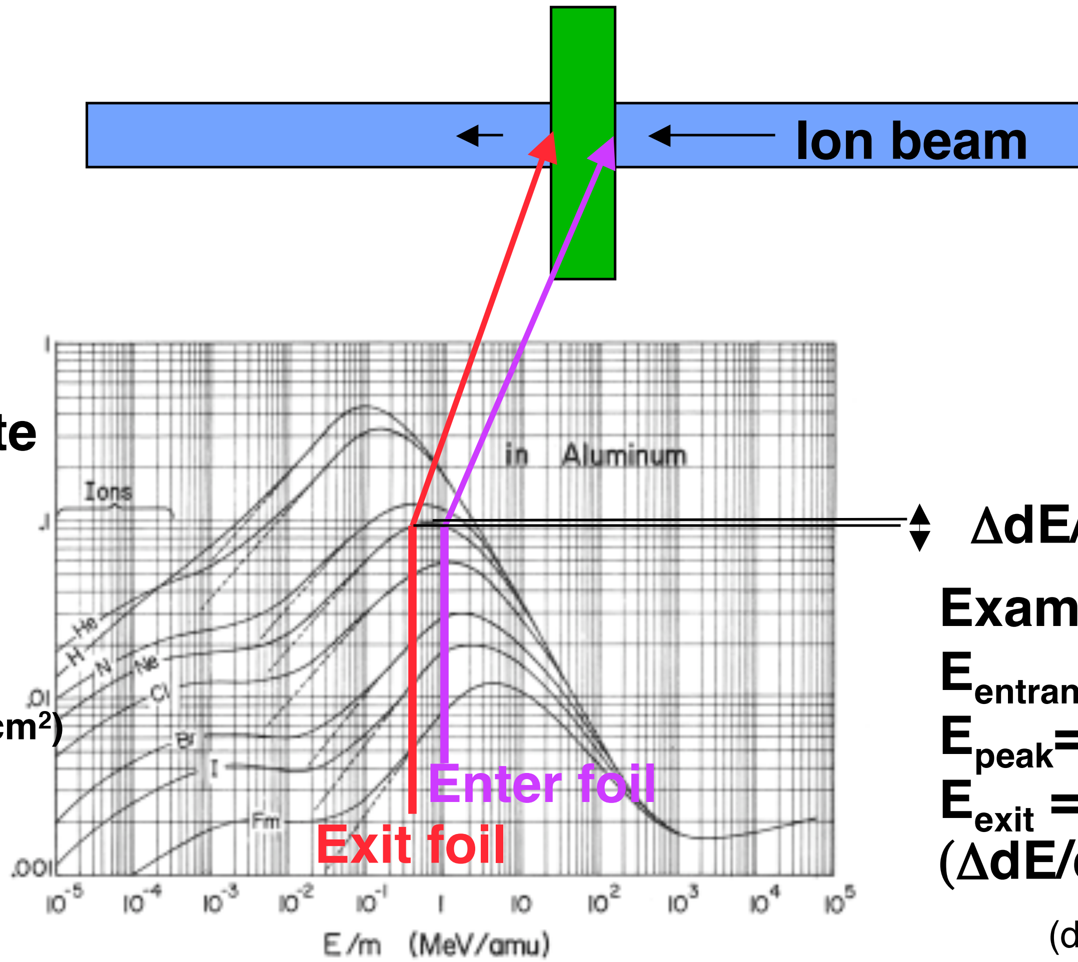
Example: ion beam deposition onto foil target (solid metal or foam)

uniformity and fractional energy loss can be high if operate at Bragg peak (Larry Grisham, PPPL)

Energy loss rate

$$-\frac{1}{Z^2}\frac{dE}{dX}$$

(MeV/mg cm^2)



Energy/Ion mass **(MeV/amu)**

$\Delta dE/dX \propto \Delta T$

Example: Neon beam
$E_{entrance}$=1.0 MeV/amu
E_{peak}= 0.6 MeV/amu
E_{exit} = 0.4 MeV/amu
$(\Delta dE/dX)/(dE/dX) \approx 0.05$

(dEdX figure from L.C Northcliffe and R.F.Schilling, Nuclear Data Tables, **A7**, 233 (1970))

The hydrodynamics of heated foils can range from simple through complex

Most idealized

Most realistic

Uniform temperature foil, instantaneously heated, ideal gas equation of state

Uniform temperature foil, instantaneously heated, realistic equation of state

Foil heated nonuniformly, non-instantaneosly realistic equation of state

Foil heated nonuniformly, non-instantaneosly realistic equation of state, and microscopic physics of droplets and bubbles resolved

The goal: use the measurable experimental quantities ($v(z,t)$, $T(z,t)$, $\rho(z,t)$, $P(z,t)$) to invert the problem: what is the equation of state, if we know the hydro?

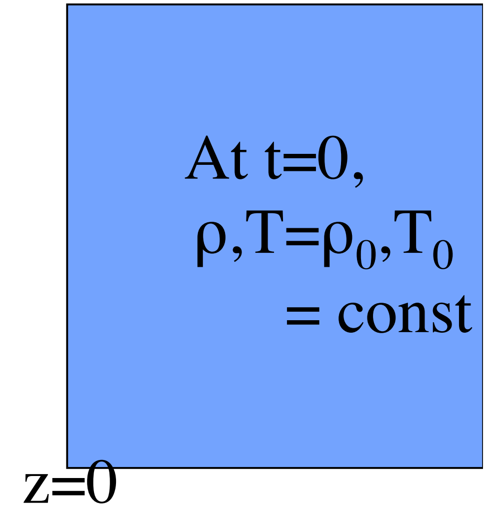
In particular, what are the "good" quantities to measure?

The problem of a heated foil may be found in fluld mechanics textbooks (e.g. Landau and Lifshitz, Fluid Mechanics or Zeldovich and Raizer, Physics of shock waves...)

$$\frac{\partial \rho}{\partial t} + \frac{\partial \rho v}{\partial z} = 0 \qquad \text{(continuity)}$$

$$\frac{\partial v}{\partial t} + v\frac{\partial v}{\partial z} = -\frac{1}{\rho}\frac{\partial p}{\partial z} \qquad \text{(momentum)}$$

$$p = K\rho^{\gamma} \qquad \text{(adiabatic ideal gas)}$$



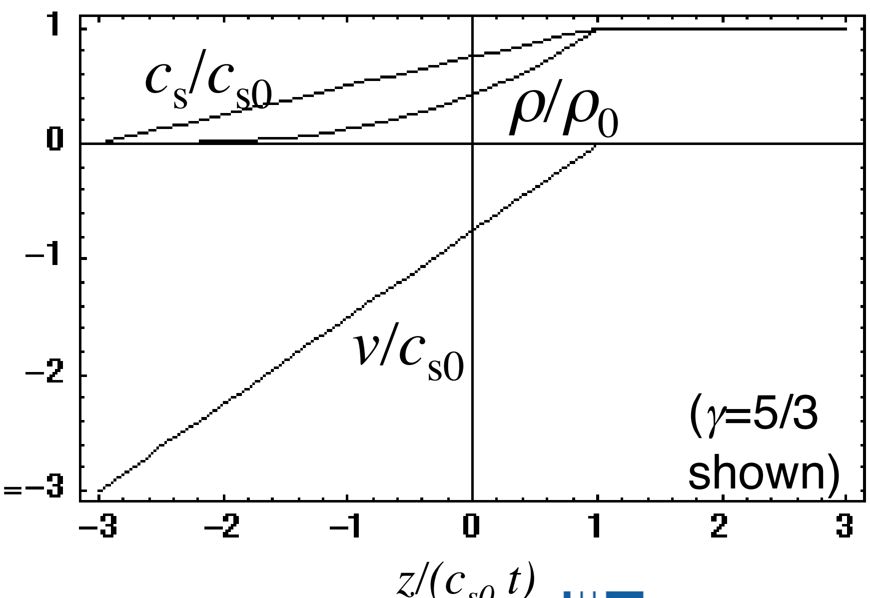
Similarity solution can be found for simple waves:

$$\frac{v}{c_{s0}} = \left(\frac{2}{\gamma+1}\right)\left(\frac{z}{c_{s0}t} - 1\right) \qquad (c_s^{\,2} \equiv \gamma P/\rho)$$

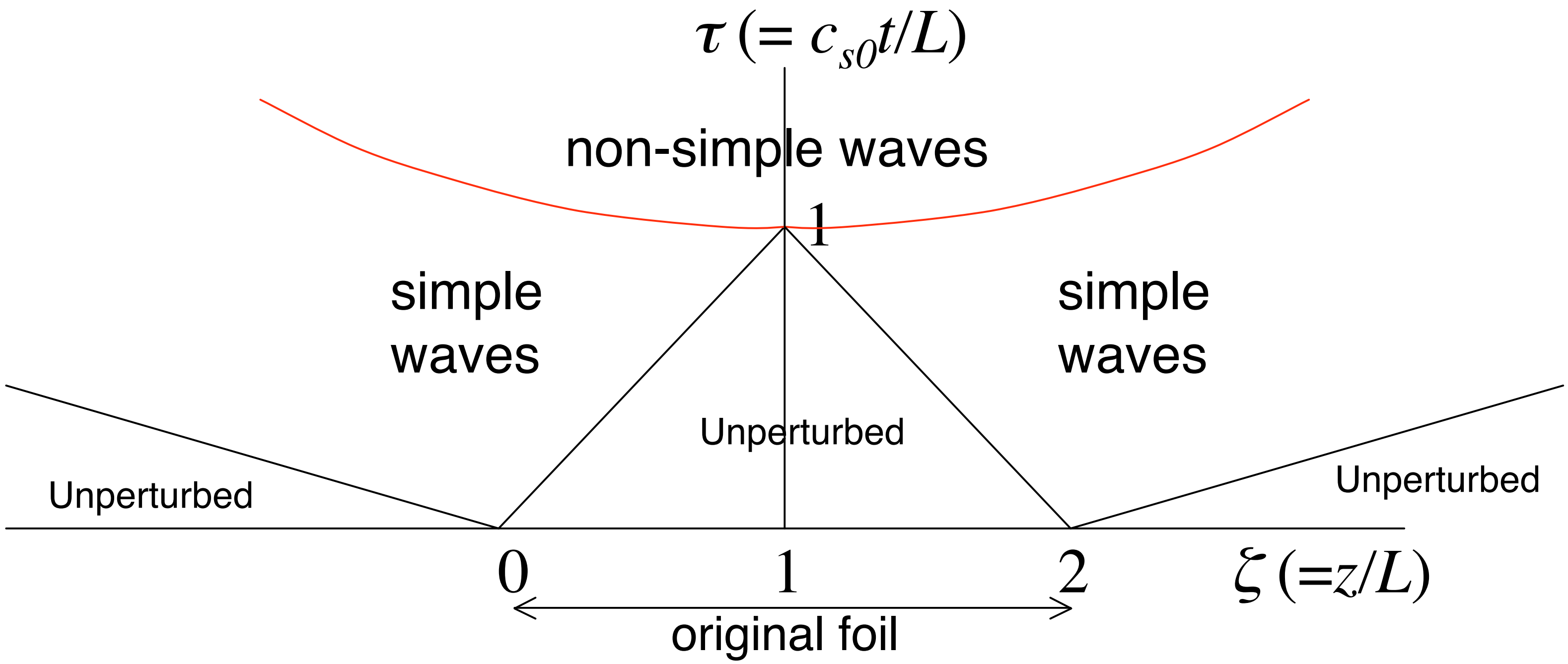
$$\frac{c_s}{c_{s0}} = \left(\frac{\gamma-1}{\gamma+1}\right)\left(\frac{z}{c_{s0}t}\right) + \frac{2}{\gamma+1};$$

$$\frac{\rho}{\rho_0} = \left(\frac{c_s}{c_{s0}}\right)^{2/(\gamma-1)}; \qquad \frac{T}{T_0} = \left(\frac{c_s}{c_{s0}}\right)^{2}$$

$$v = \frac{-2}{\gamma-1}c_{s0} = -3$$



Simple wave solution good until waves meet at center; complex wave solution is also found in LL textbook



Using method of characteristics
LL give boundary between simple and complex waves:

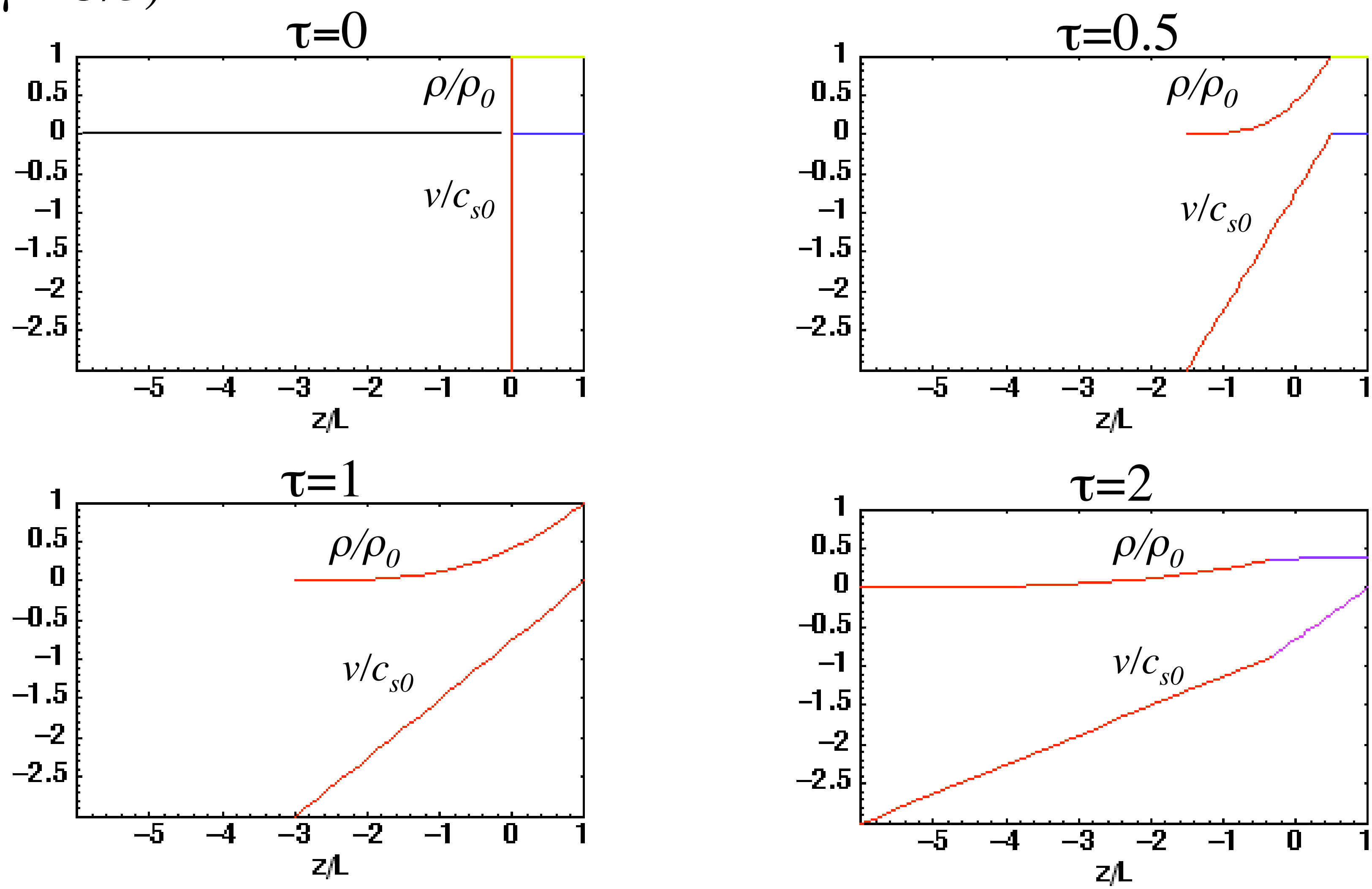
$$\zeta = \frac{-2}{(\gamma-1)}\tau + \left(\frac{\gamma+1}{\gamma-1}\right)\tau^{\frac{3-\gamma}{\gamma+1}} \qquad (\text{for } \tau>1)$$

where $\zeta \equiv z/L$ and $\tau \equiv c_{s0}t/L$

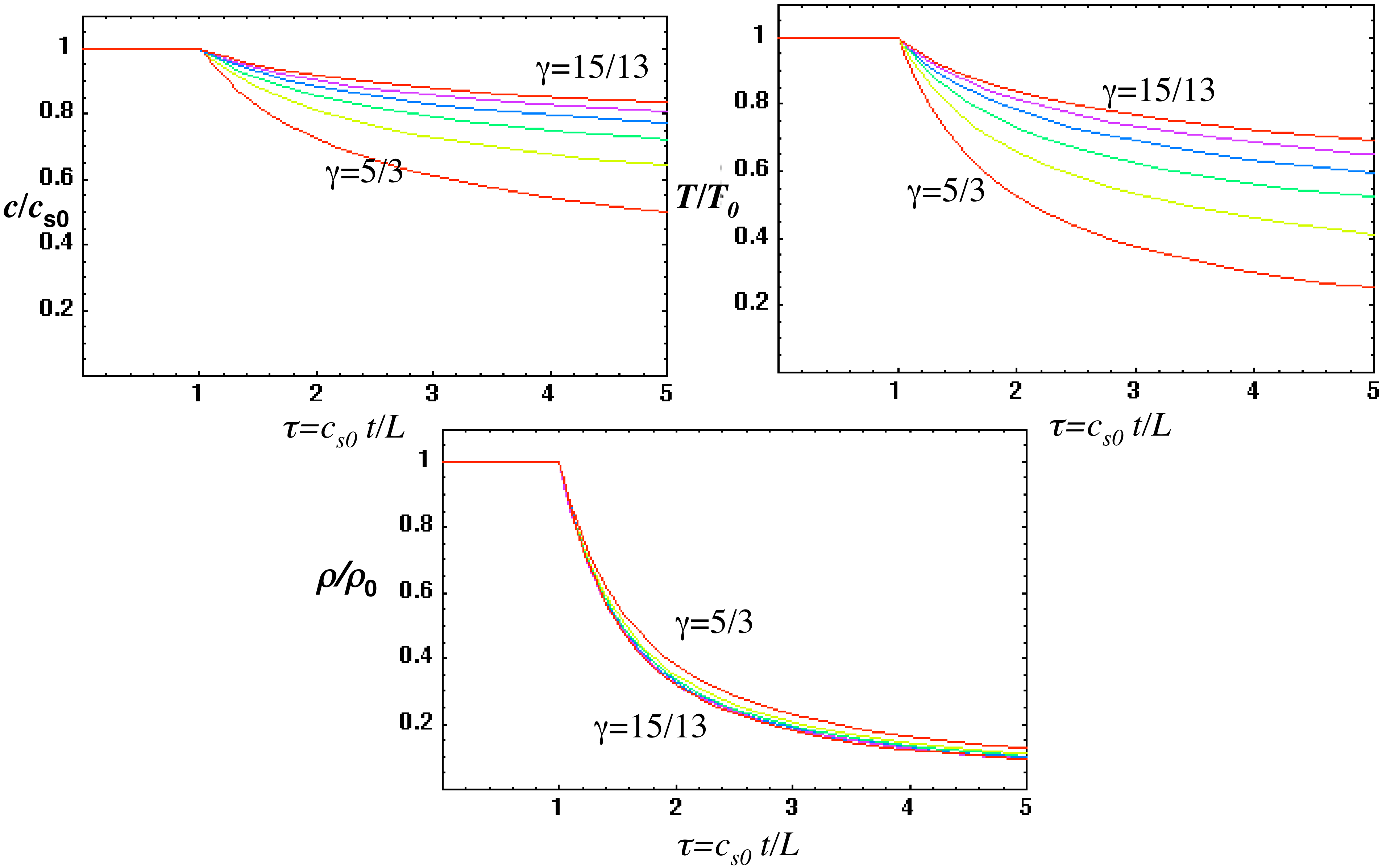
Similarity solution: snapshots of density and velocity

($\gamma = 5/3$)

(Half of space shown, $\tau = c_{s0}t/L$)



Time evolution of central T, ρ, and c_s for γ between 5/3 and 15/13



Similarity solution may be found for more complicated EOS. Solution is reduced to ODE[1,2,3].

$$\frac{\partial \rho}{\partial t} + \frac{\partial \rho v}{\partial z} = 0$$ **continuity**

$$\frac{\partial v}{\partial t} + v\frac{\partial v}{\partial z} = -\frac{1}{\rho}\frac{\partial p}{\partial z}$$ **momentum**

Let $P \equiv v + I$ **and** $M \equiv v - I$ **where** $I(\rho) \equiv \int_{\rho_0}^{\rho} \frac{c_s(\rho')}{\rho'} d\rho'$

and where $c_s^{\,2}(\rho) \equiv \left.\frac{\partial p}{\partial \rho}\right|_s$

The continuity and momentum equation can be transformed to:

$$\frac{\partial P}{\partial t} + (v + c_s)\frac{\partial P}{\partial z} = 0 \qquad \frac{\partial M}{\partial t} + (v - c_s)\frac{\partial M}{\partial z} = 0$$

There is no natural time or space scale to the problem. This suggests trying a similarity variable. Let $\xi \equiv z/(c_{s0}t)$

Then the partial derivatives $\frac{\partial P}{\partial t} = P'(\xi)\frac{\partial \xi}{\partial t} = -P'(\xi)\frac{\xi}{t}$ **and** $\frac{\partial P}{\partial z} = P'(\xi)\frac{\xi}{z}$

The equations for P **and** M **then become:**

$$(v + c_s - \xi c_{s0})P'(\xi) = 0 \quad \textbf{and} \quad (v - c_s - \xi c_{s0})M'(\xi) = 0$$

1. Zelodovich and Raizer, "Physics of High Temperature Hydodynamics Phenomena," (1962) 2. Anisimov, S.I. et al, Applied Physics A 69, 617 - 620 (1999) 3. R. More, T. Kato, H.Yoneda, NIFS Report (2005)

Similarity solution -- continued

The solutions are then trivial:

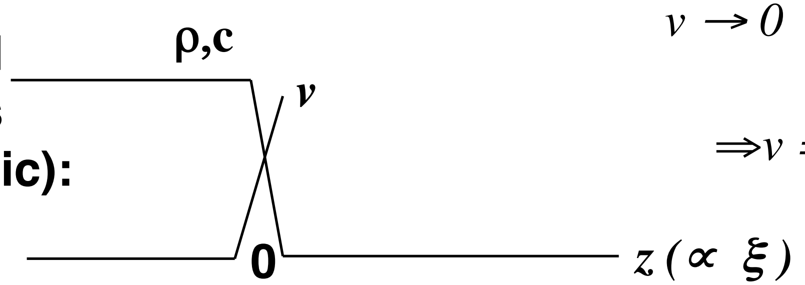
$v = \xi c_{s0} - c_s$ **and** $M'(\xi) = 0$ **or** $v = \xi c_{s0} + c_s$ **and** $P'(\xi) = 0$

Consider the conditions at t near 0.

$c_s \to 0$ when $v > 0$ and $\xi > 0$ (doesn't help choose)

$v \to 0$ when $c_s > 0$ and $\xi < 0$ (rules out 1st solution)

Expected solutions (schematic):



$\Rightarrow v = \xi c_{s0} + c_s$ **and** $P'(\xi) = 0$ **for this configuration**

$P'(\xi) = 0 \Rightarrow P(\xi) = constant$ **or** $v = -I(\rho) + constant$. **Since** $v=0$ **when** $\rho=\rho_0$, **the** $constant = 0$.

So the full solution is:

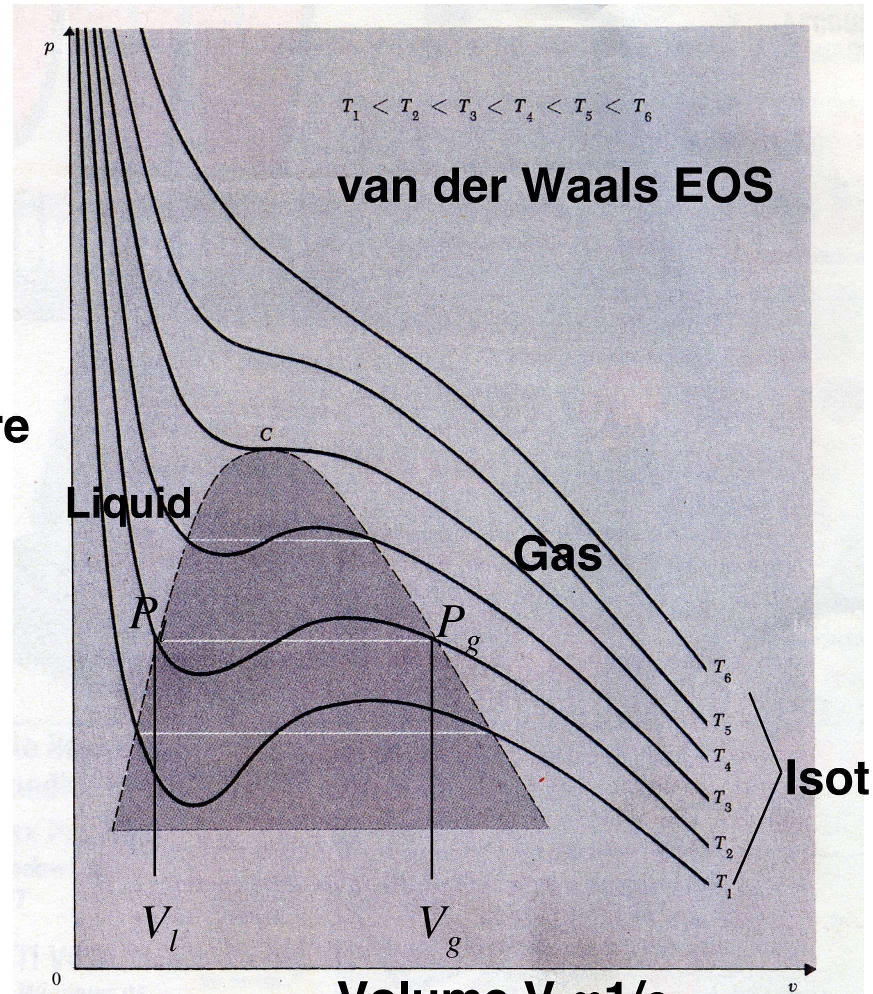
$\xi c_{s0} = -I(\rho) - c_s(\rho)$ **implicitly gives** ρ **as a function of the coordinate** $\xi \equiv z/(c_{s0}t)$

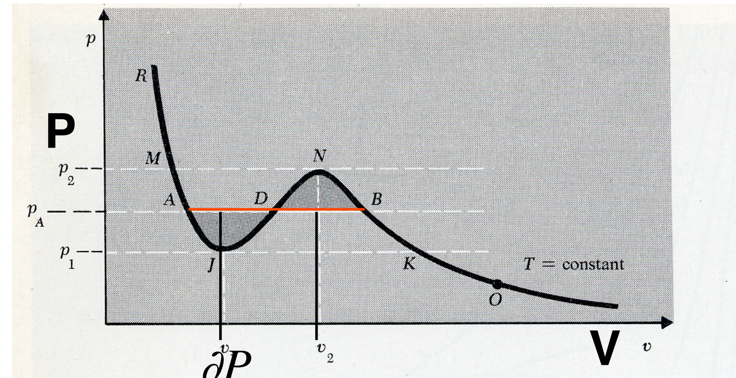
$v = -I(\rho)$ **and** $c_s(\rho)$ **are then also implictly functions of** ξ

The trick is to be able to calculate $c_s^2(\rho) \equiv \left.\dfrac{\partial p}{\partial \rho}\right|_s$ **and** $I(\rho) \equiv \int_{\rho_0}^{\rho} \dfrac{c_s(\rho')}{\rho'} d\rho'$

For a perfect gas: $c_s^2(\rho) = \dfrac{\gamma P_0}{\rho_0}\left(\dfrac{\rho}{\rho_0}\right)^{\gamma-1}$ **and the integral for** $I(\rho)$ **may be carried out.**

For a van der Waals EOS, the sound speed can become imaginary, so Maxwell (equilibrium) construction is used instead





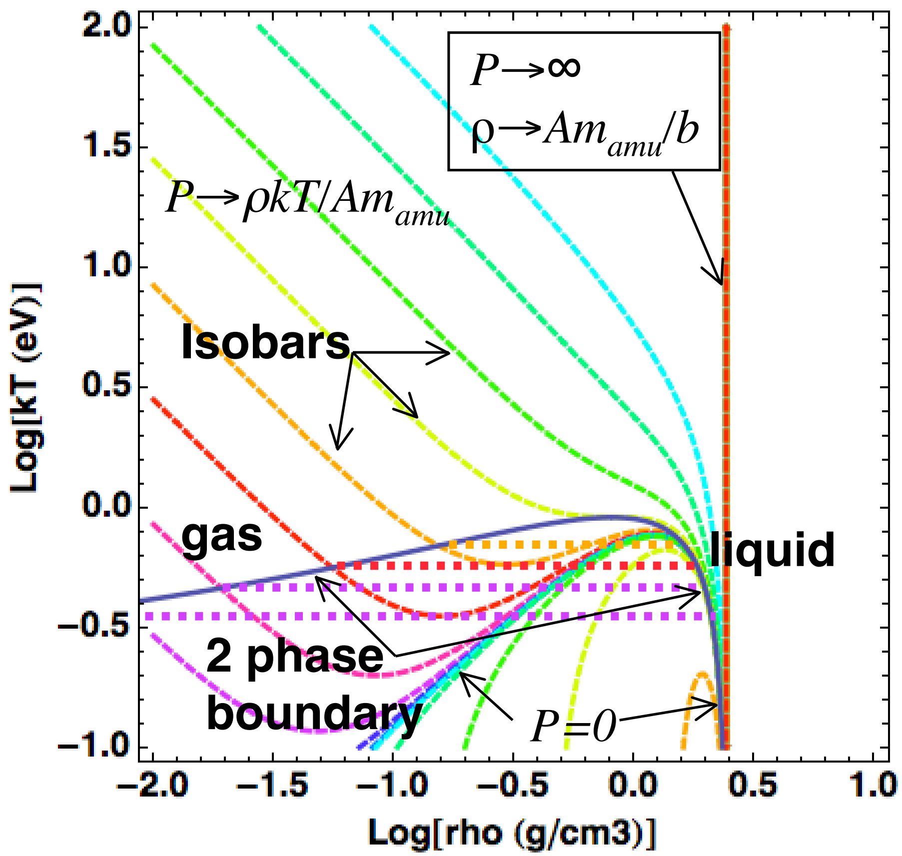
$$\frac{\partial P}{\partial V} > 0 \;\rightarrow\; \textbf{instability}$$

Maxwell construction replaces unstable region on isotherm curve with constant pressure 2-phase region where liquid and vapor coexist

The liquid/gas border is determined by demanding $p_l = p_g$ **and** $\int_{V_l}^{V_g}(p - p_g)dV = 0$
The latter condition is equivalent to the liquid and gas having the same Gibbs Free Energy $G = TS - \varepsilon - pV$

(Figures from F. Reif, "Fundamentals of statistical and thermal physics")

With Maxwell construction, sound speed is real, and $I(\rho)$ integral may be carried out



Mass fraction of gas (x_g) and liquid (x_l):

$$x_g = \rho_g V_g / (\rho V) \qquad x_l = \rho_l V_l / (\rho V)$$

$$V_g + V_l = V \qquad \rho_g V_g + \rho_l V_l = \rho V$$

$$\Rightarrow \quad x_l(\rho,T) = \frac{\rho_l(T)}{\rho}\left(\frac{\rho - \rho_g(T)}{\rho_l(T) - \rho_g(T)}\right)$$

and $x_g(\rho,T) = 1 - x_l(\rho,T)$

$$s(\rho,T) = x_l(\rho,T)s(\rho_l(T),T) + x_g(\rho,T)s(\rho_g(T),T)$$

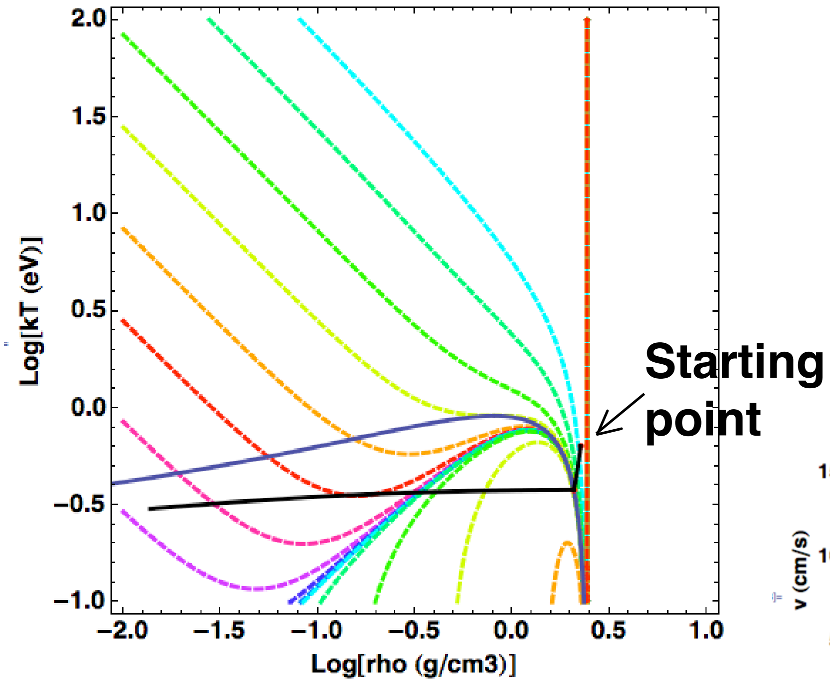
On isentrope $s(\rho,T)$ = initial entropy s_0 so:

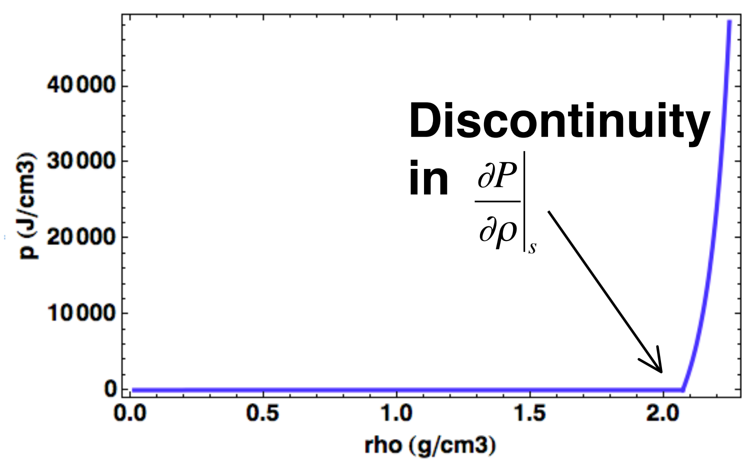
$$x_l(T) = \frac{s_0 - s_g(T)}{s_l(T) - s_g(T)} \quad ; \quad \rho(T) = \frac{\rho_l(T)\rho_g(T)}{x_g(T)\rho_l(T) + x_l(T)\rho_g(T)}$$

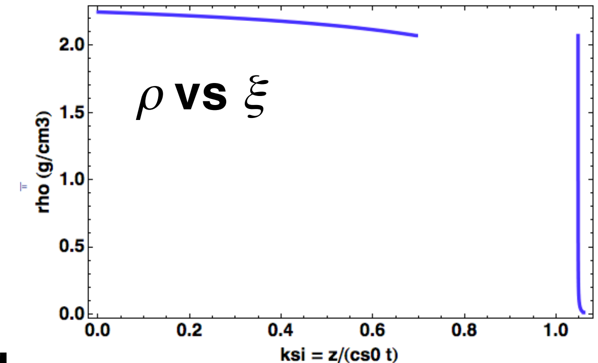
$$p(T) = p(\rho_l(T),T) = p(\rho_g(T),T)$$

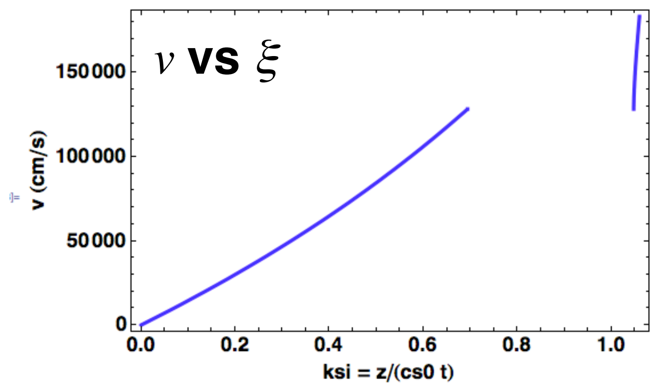
So $$c_s^2 = \left.\frac{\partial P(s,\rho)}{\partial \rho}\right|_s = \frac{\dfrac{dp(T)}{dT}}{\dfrac{d\rho(T)}{dT}}$$

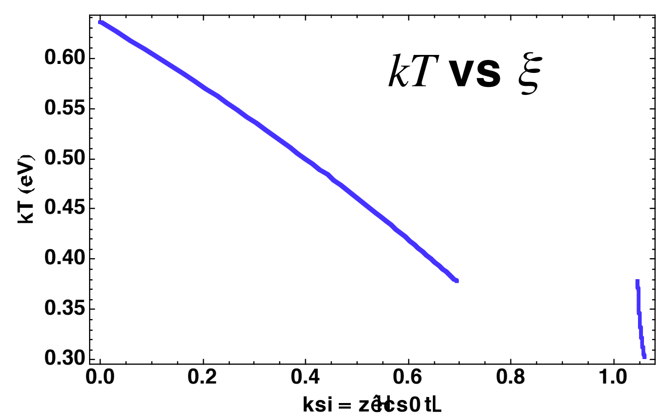
Similarity solution results with Van der Waal's EOS (with Maxwell construction)











Recall:

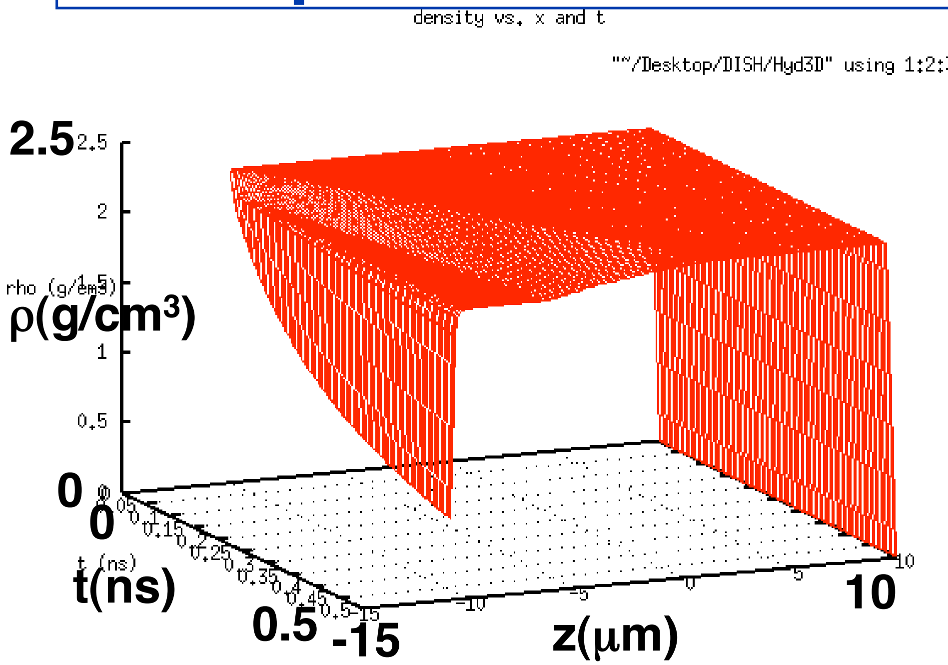
$$\xi c_{s0} = -I(\rho) - c_s(\rho)$$

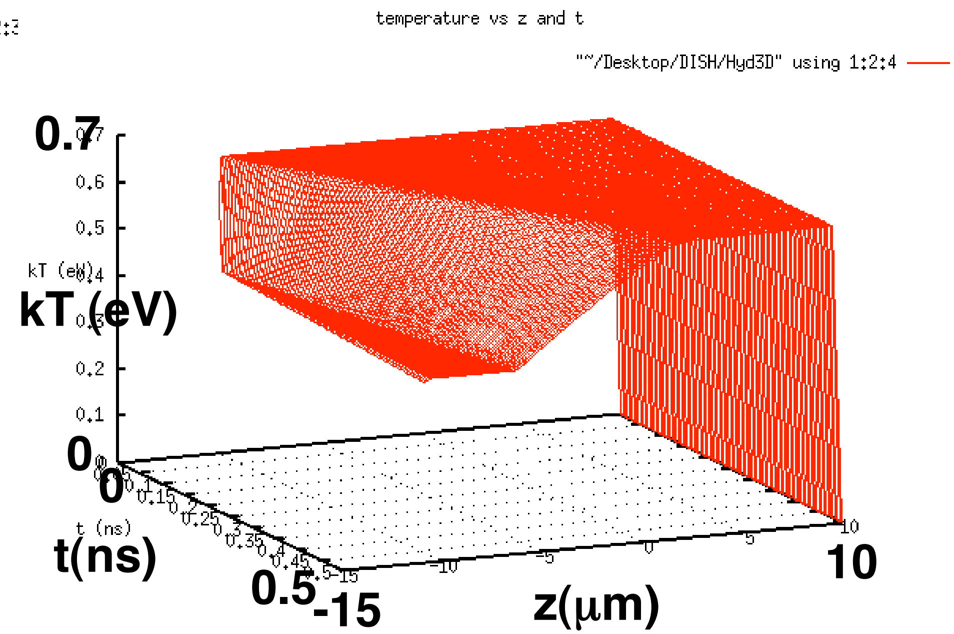
$$I(\rho) \equiv \int_{\rho_0}^{\rho} \frac{c_s(\rho')}{\rho'} d\rho'$$

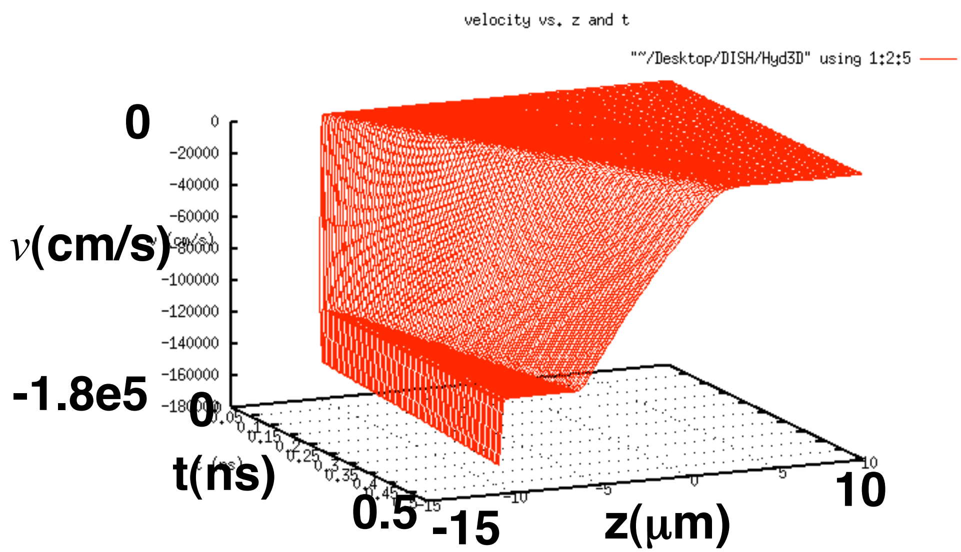
The discontinuity in c_s leads to a discontinuity in ξ in the solution for ρ, v, and kT, which are continuous

At a fixed time, this translates into "plateau's" in these quantities

R. More's code DISH shows these plateaus when plotted as function of z and t







(foil expanding to left in this simulation, so velocities <0, and edge initially at -10 μm).

Simulation codes needed to go beyond similarity solution results

Some examples used in this lecture:

DPC: 1D

- **EOS based on tabulated energy levels, Saha equation, melt point, latent heat**
- **Tailored to Warm Dense Matter regime**
- **Maxwell construction**
- **Ref: R. More, H. Yoneda and H. Morikami, JQSRT 99, 409 (2006).**

DISH: 1D, perfect gas or Van der Waals EOS

- **Ref: R. More, DISH User Manual**

HYDRA: 1, 2, or 3D

- **EOS based on:**
  - **QEOS: Thomas-Fermi average atom e-, Cowan model ions and Non-maxwell construction**
  - **LEOS: numerical tables from SESAME**
  - **Maxwell or non-maxwell construction options**
  - **Ref: M. M. Marinak, G. D. Kerbel, N. A. Gentile, O. Jones, D. Munro, S. Pollaine, T. R. Dittrich, and S. W. Haan, Phys. Plasmas 8, 2275 (2001).**

Plateaus persist in more realistic EOS based on Saha equation, using maxwell construction

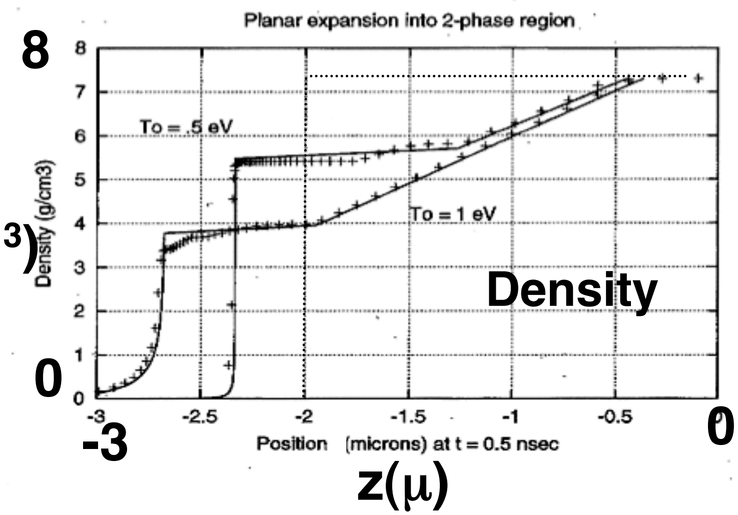
Expansion into 2-phase region leads to ρ-T plateaus with sharp edges[1,2]

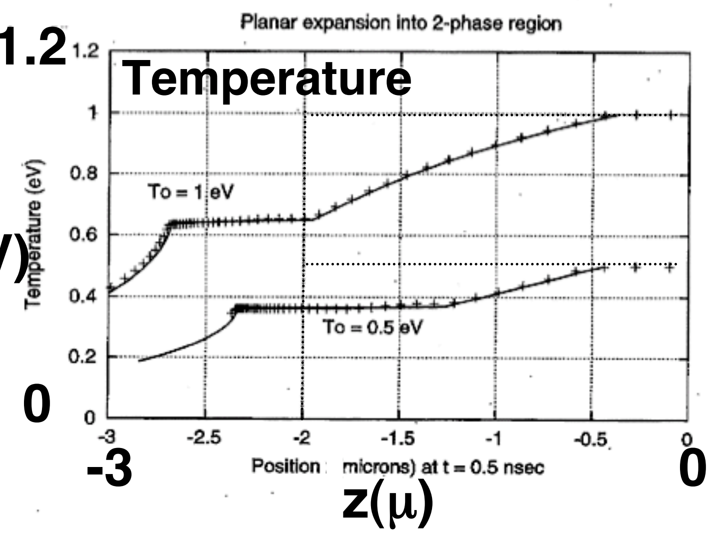
Initial distribution (dotted line)

Exact analytic hydro (using numerical EOS) (solid line)

+++++++++ Numerical hydro

DPC code results:



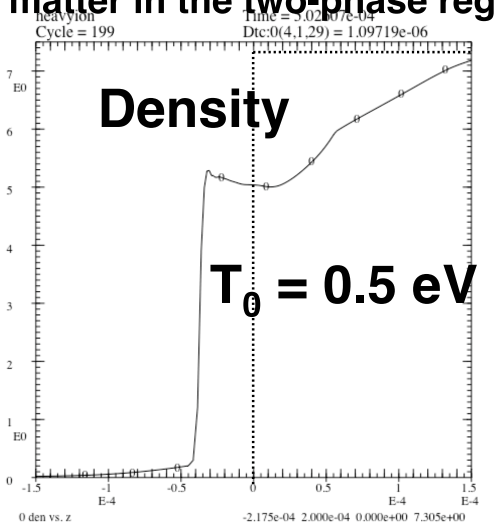


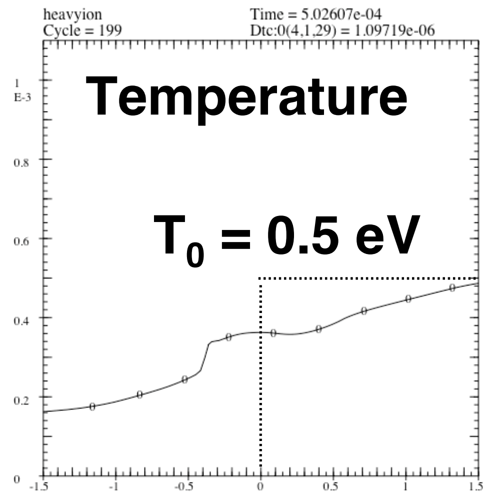
Example shown here is initialized at T=0.5 or 1.0 eV and shown at 0.5 ns after "heating."

[1]More, Kato, Yoneda, NIFS Report (2005). [2]Sokolowski-Tinten et al, PRL 81, 224 (1998)

HYDRA simulations show both similarities to and differences with More, Kato, Yoneda simulation of 0.5 and 1.0 eV Sn at 0.5 ns

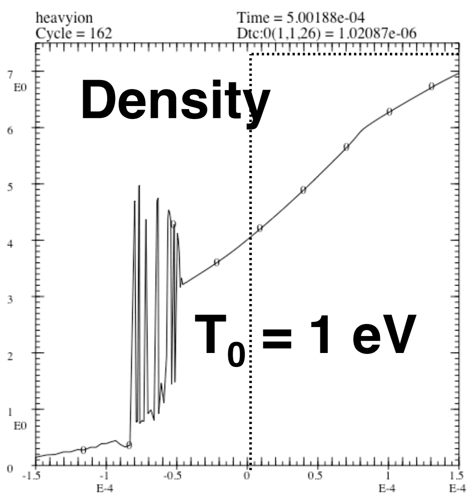
(oscillations at phase transition at 1 eV are physical/numerical problems, triggered by the different EOS physics of matter in the two-phase regime)

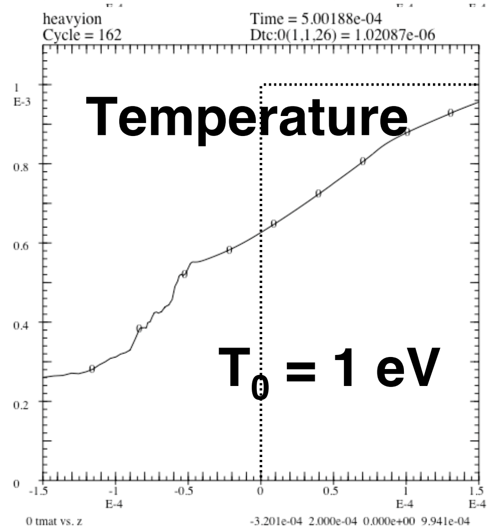




Propagation distance of sharp interface is in approximate agreement

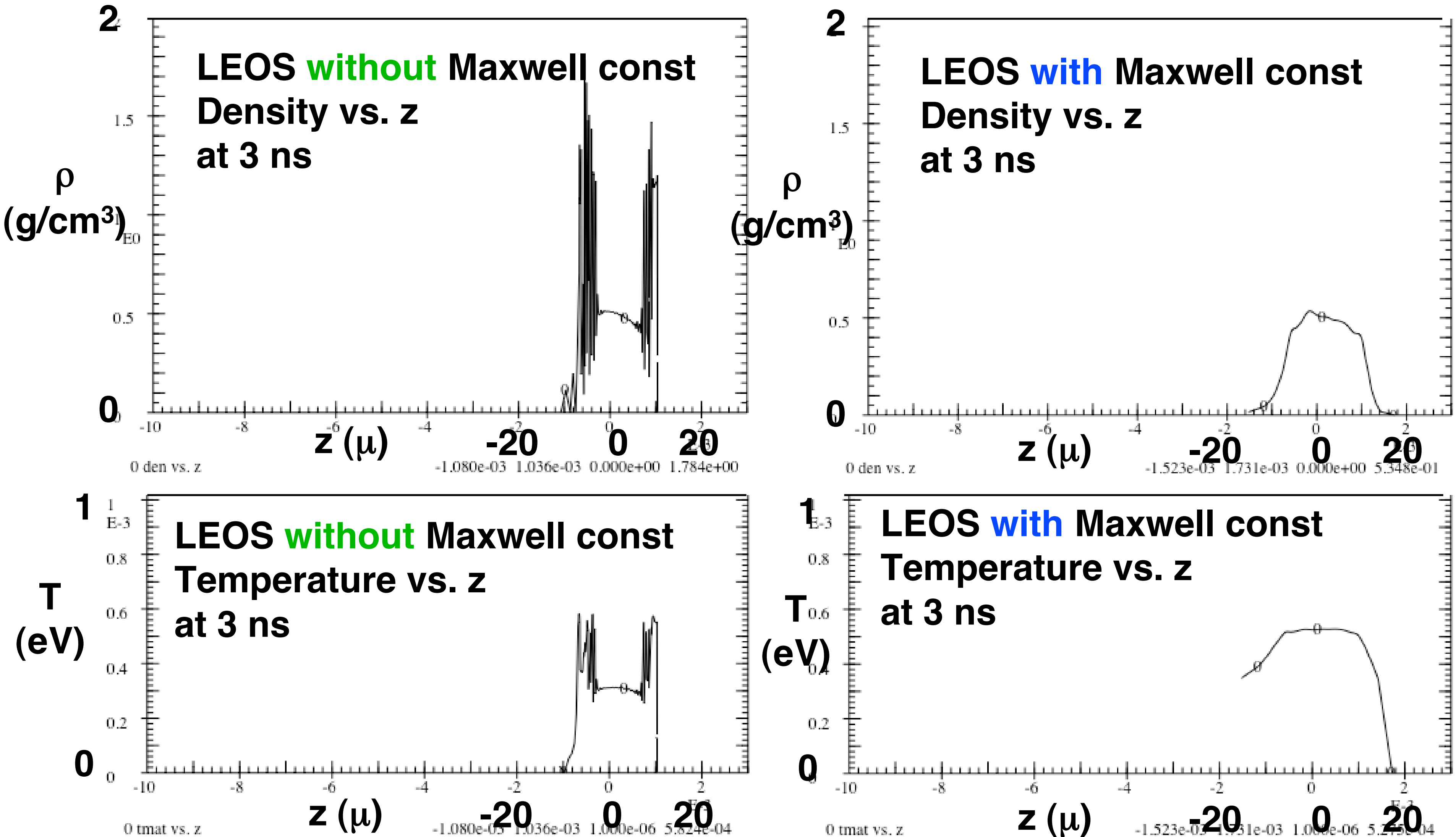
Density oscillation likely caused by $\partial P/\partial \rho$ instabilities, (bubbles and droplets forming?)





Uses QEOS with no Maxwell construction

Maxwell construction reduces instability in numerical calculations



All four plots: HYDRA, 3.5 μ foil, 1 ns, 11 kJ/g deposition in Al target

Parametric studies

Case study: possible option for NDCX II

2.8 MeV Lithium$^+$ beam

Deposition 20 kJ/g

1 ns pulse length

3.5 micron solid Aluminum target

Varied: foil thickness

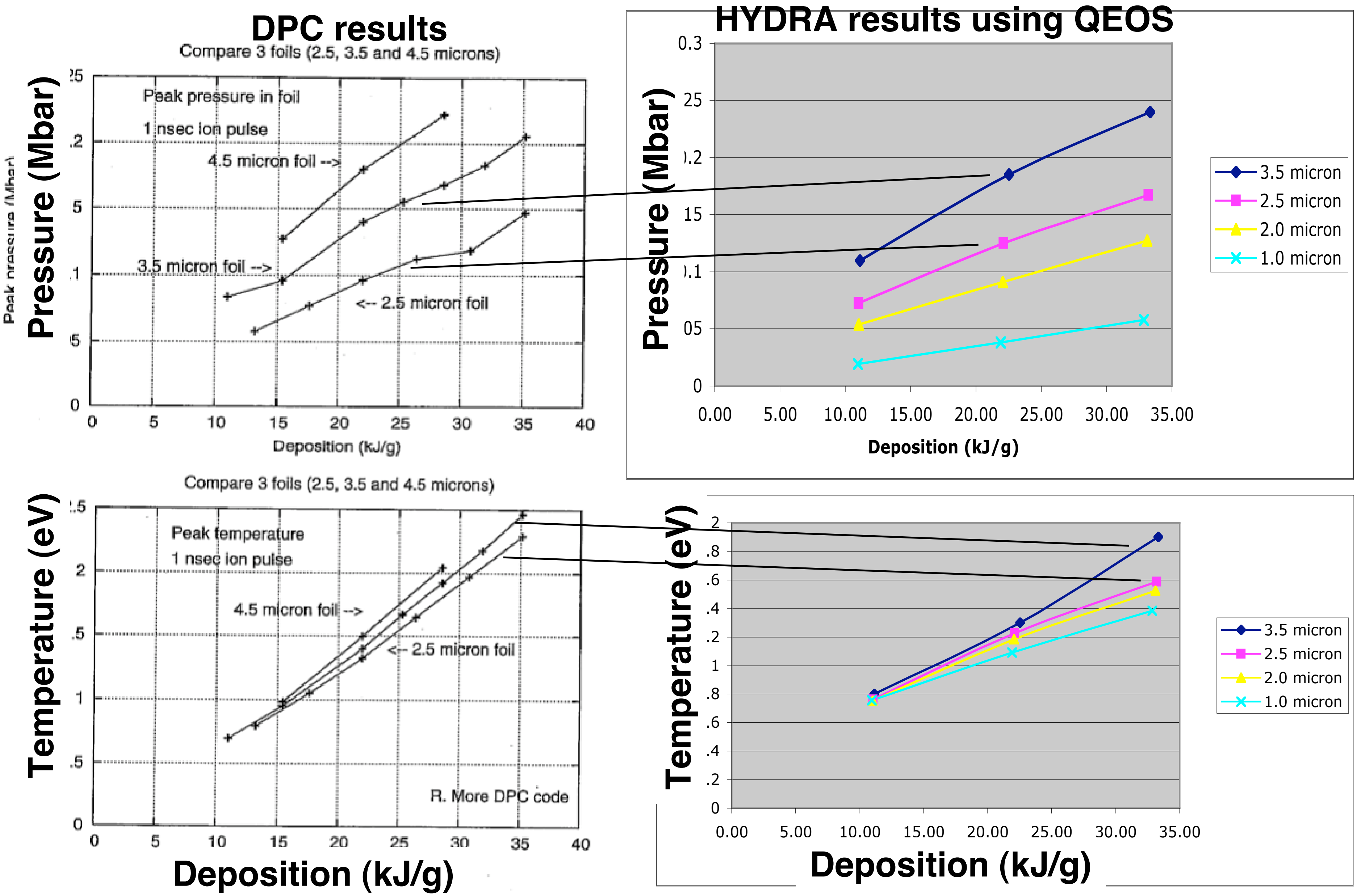
finite pulse duration

beam intensity

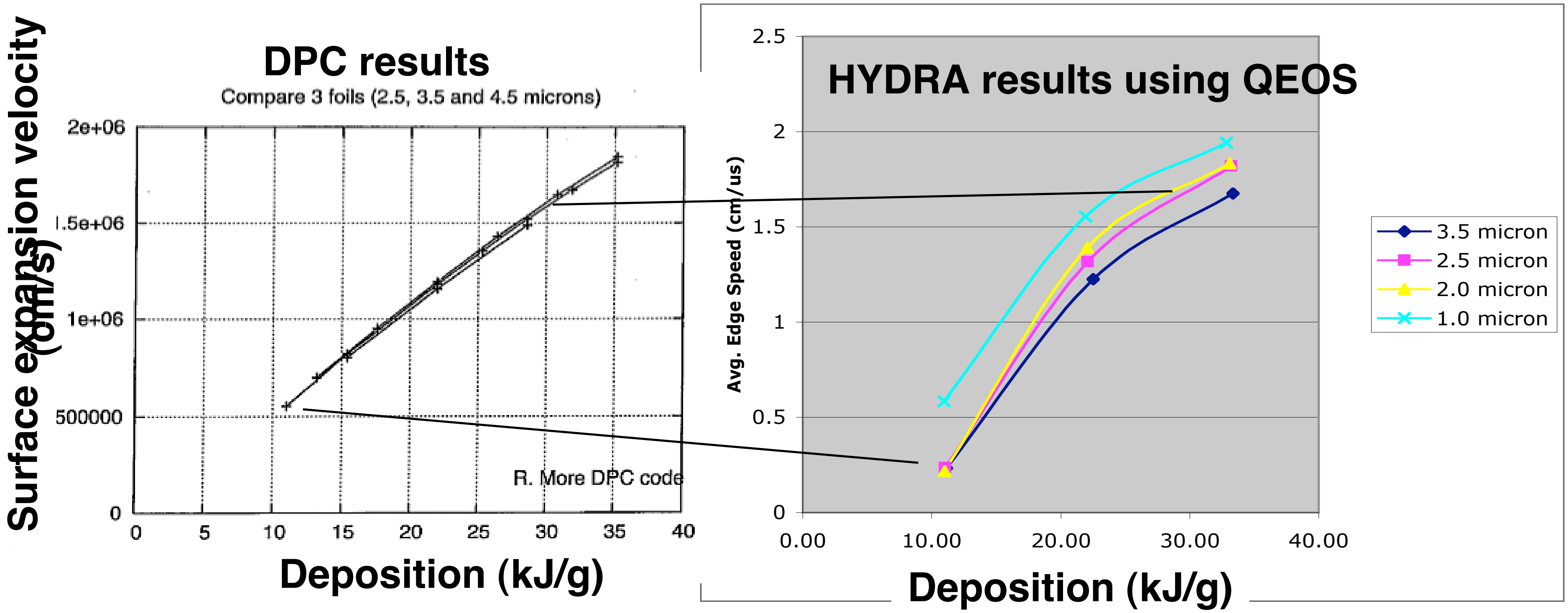
EOS/code

Purpose: gain insight into future experiments

Variations in foil thickness and energy deposition



Expansion velocity is closely correlated with energy deposition but also depends on EOS



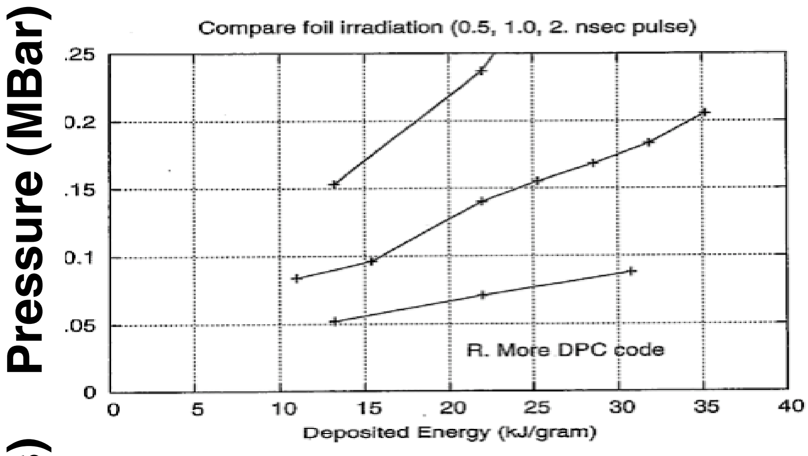
Returning to model found in text books:

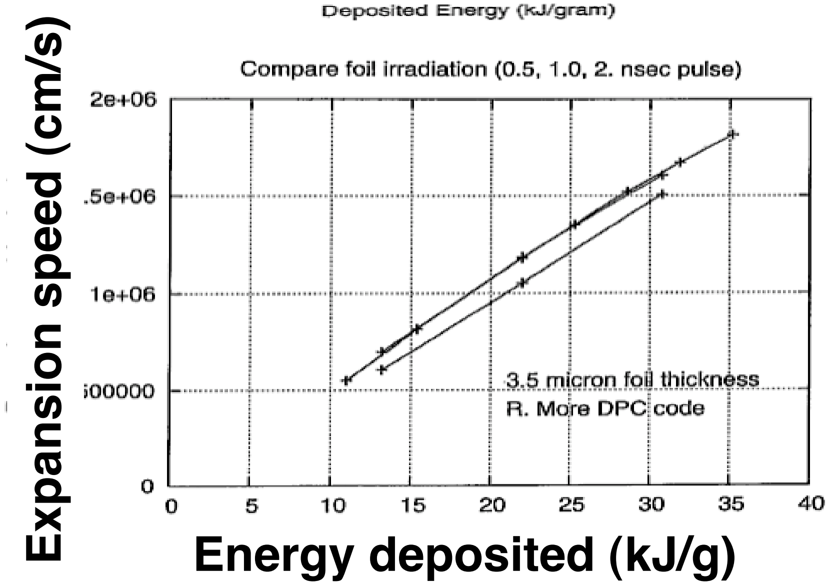
$$\varepsilon_0 = \frac{c_{s0}^2}{\gamma(\gamma-1)} \qquad v = \frac{-2c_{s0}}{\gamma-1} \qquad \Longrightarrow \qquad v = \sqrt{\frac{4\gamma}{\gamma-1}\varepsilon_0^{1/2}}$$

In instanteneous heating/perfect gas model outward expansion velocity depends only on ε_0 and γ

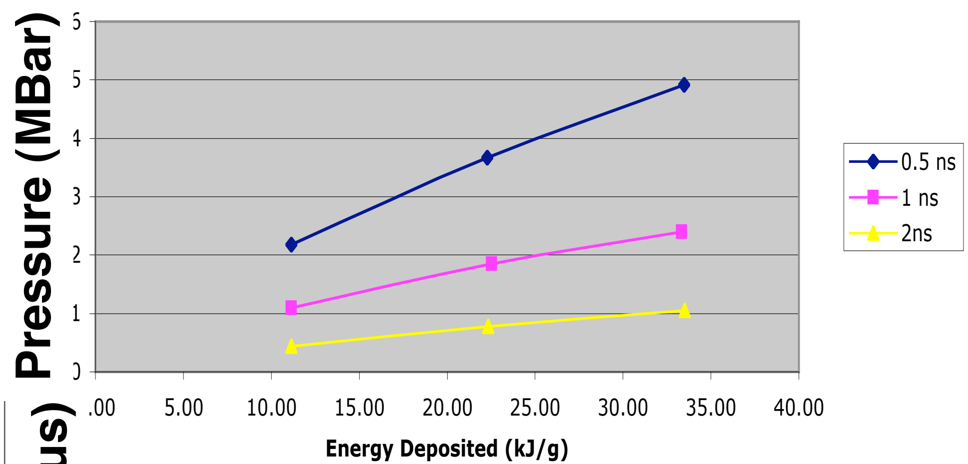
Pulse duration scaling shows similar trends

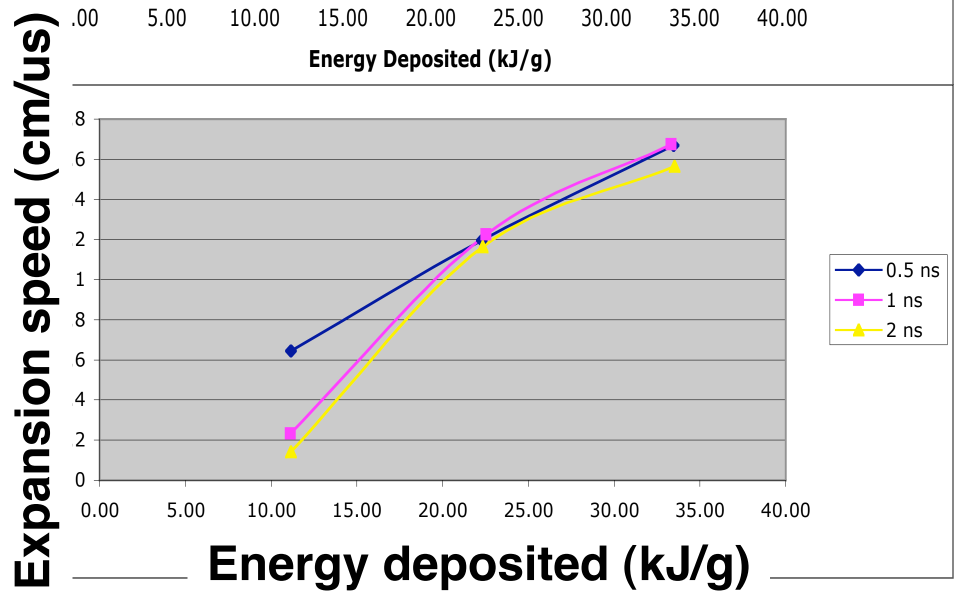
DPC results



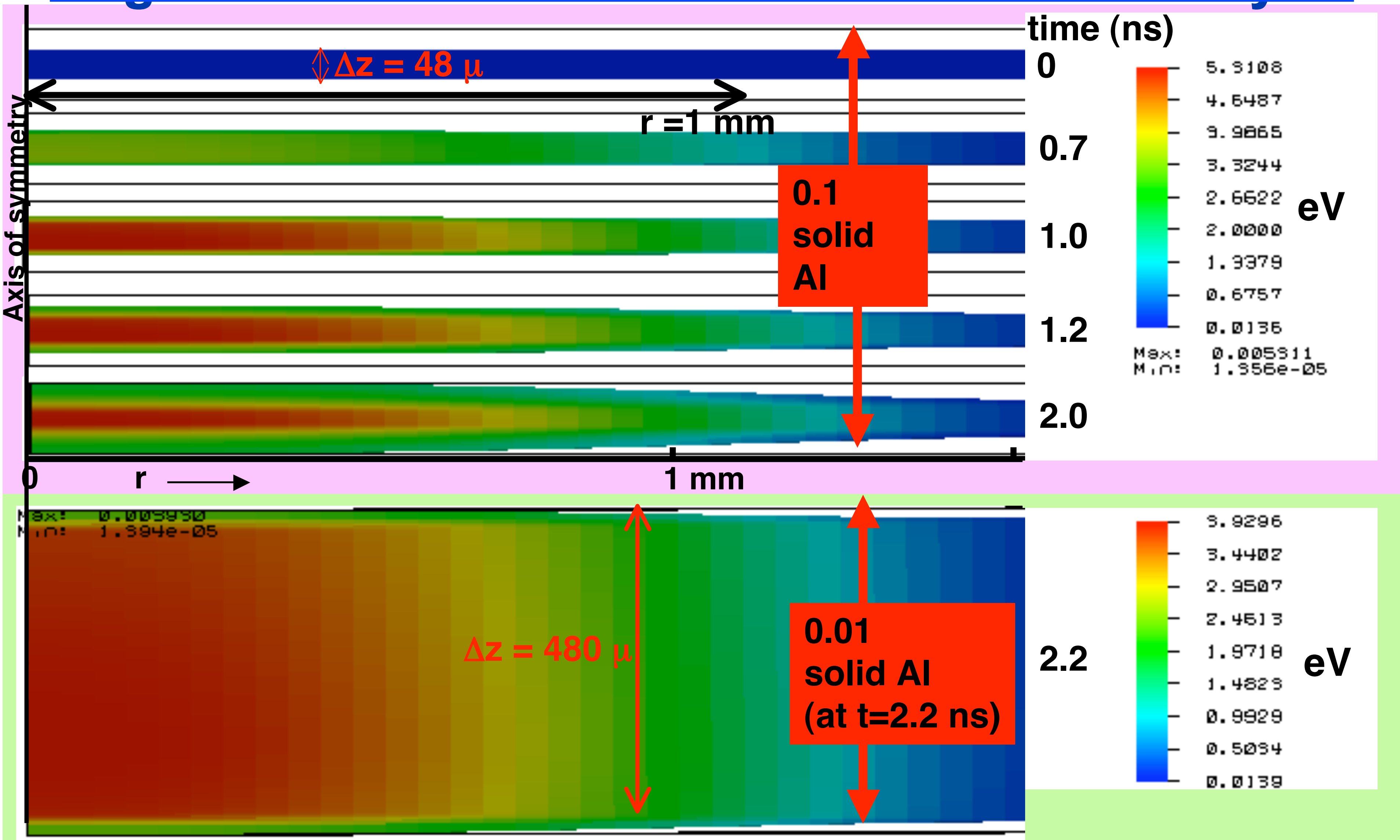


HYDRA results using QEOS



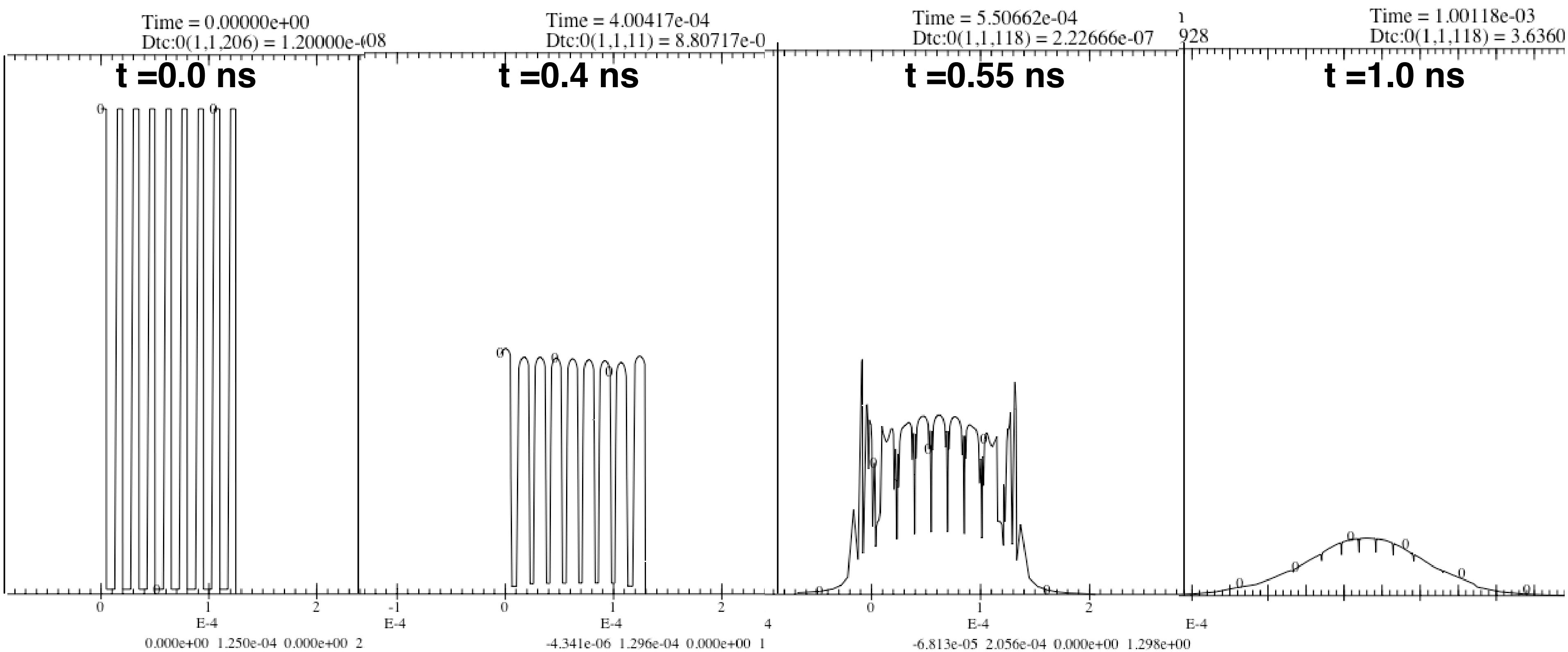


Metalic foams are being considered for WDM targets. HYDRA simulations confirm uniformity.



(simulations for 0.3 μC, 20 MeV Ne beam -- possible NDCX II / IB HEDPX parameters).

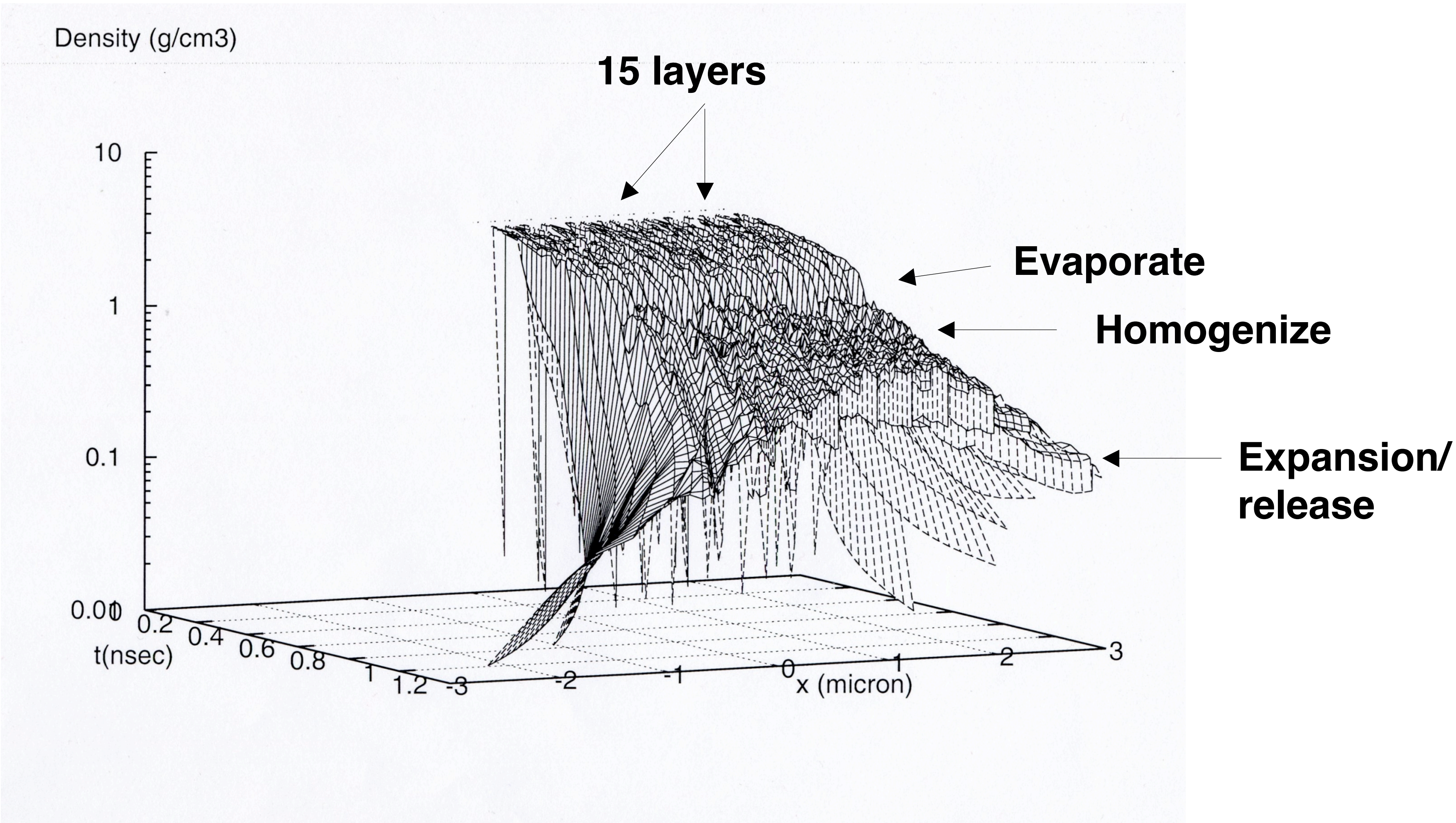
We simulate foams as multiple layers (solid density interspersed with low density voids)



density vs position
average density = 0.33 solid density

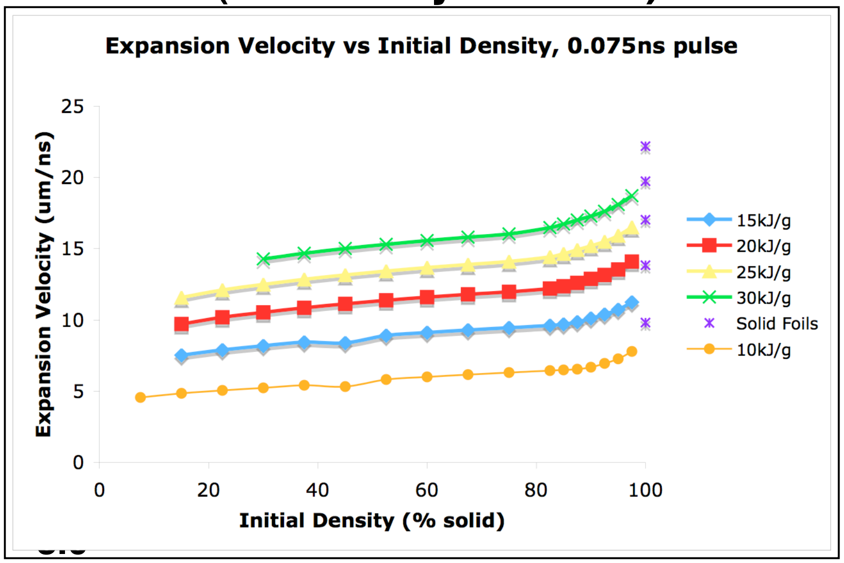
Studies being carried out using HYDRA and DPC/DISH (R. More).

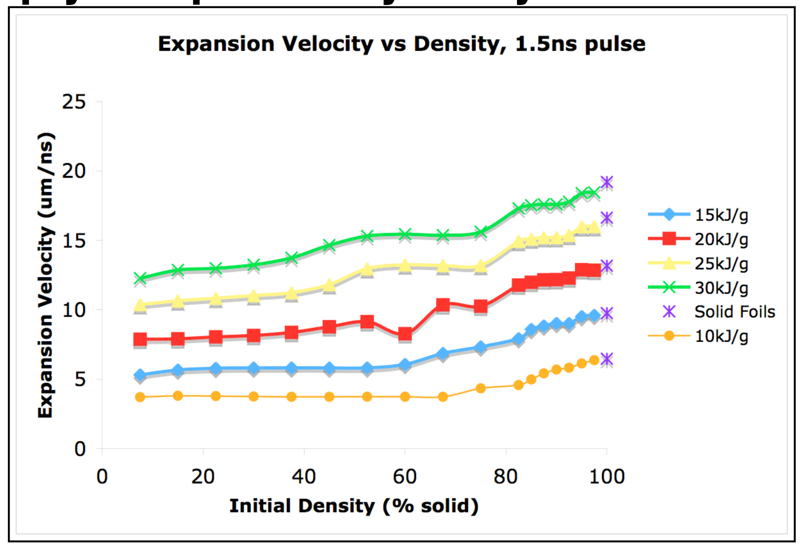
Using DPC with Saha-based EOS or DISH with van der Waals EOS, qualitatively similar results are obtained

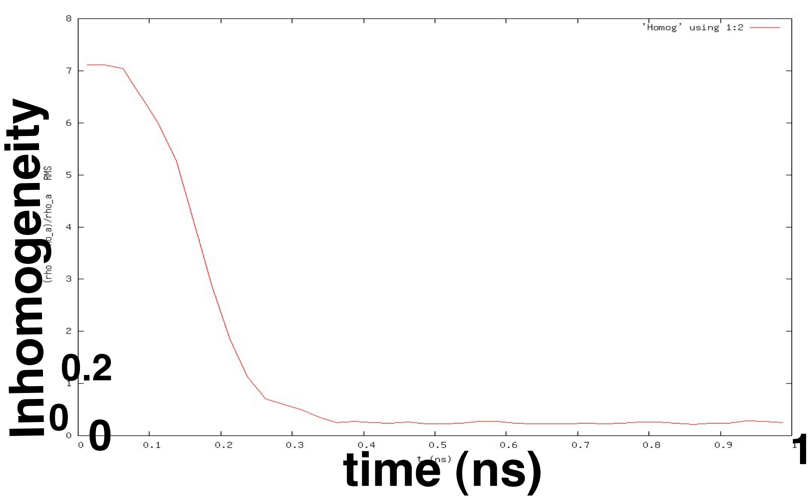


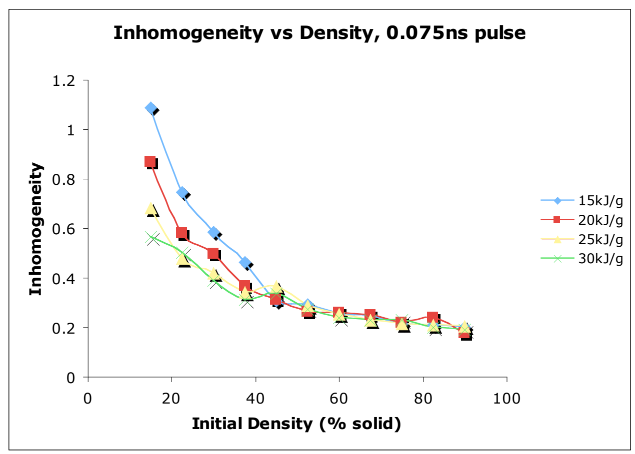
Simulations using 1D code DISH using van der Waals EOS have been exploring systematic trends of heated 1D foams

DISH (written by R. More) is a "Deeply Simplified Hydrodynamics" code.









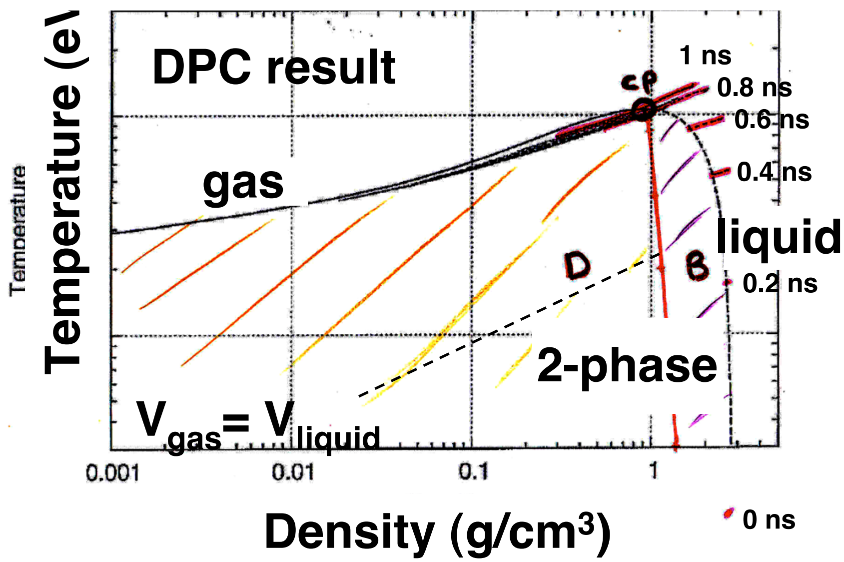
Study was carried out by A. Zylstra et al, 2007. See Friday poster.

Van der Waals EOS used.

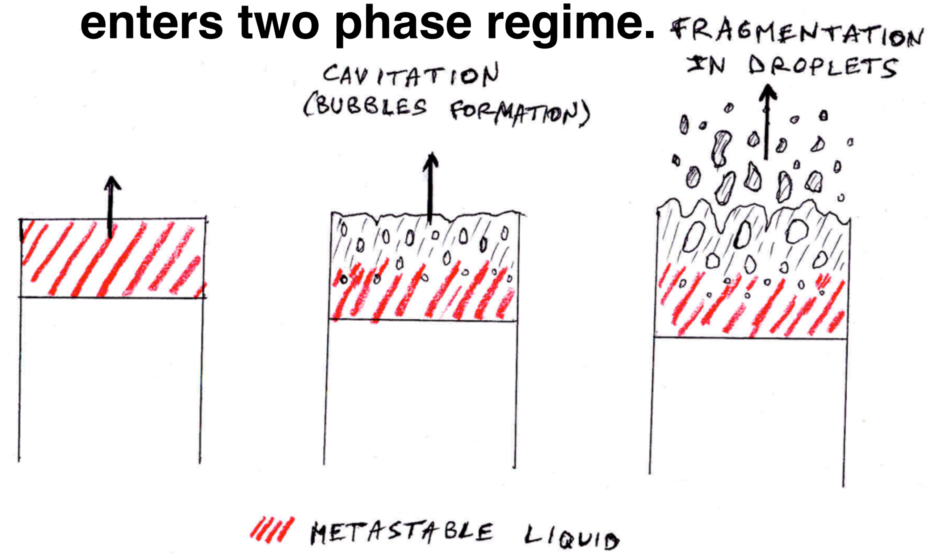
$$p = \frac{\rho k T}{A m_{amu}(1 - b\rho)} - a\rho^2$$

Formation of droplets during expansion of foil is being investigated using a kinetic code

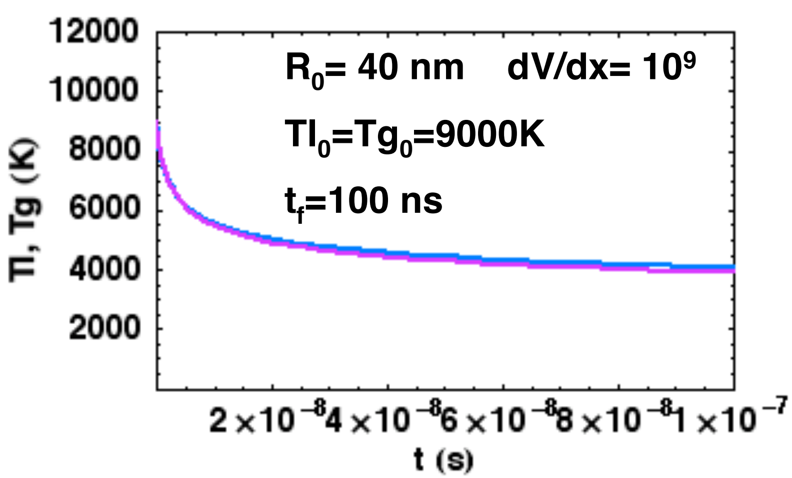
Example of evolution of foil in ρ and T

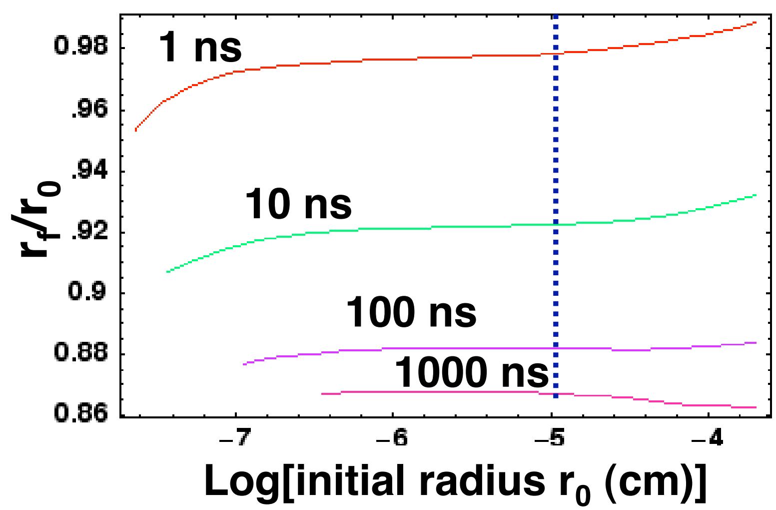


Foil is first entirely liquid then enters two phase regime.

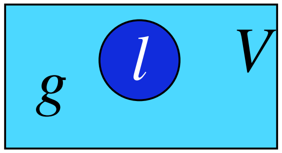


(Ref: J. Armijo, master's internship report, ENS, Paris, 2006; Armijo et al APS DDP 2006, and in prep.)





Kinetic equations: 4 variables, 4 equations



=volume of gas + liquid drop

N_l, T_l = number of particles, temperature of liquid drop;
N_g, T_g = number of particles, temperature of gas

α = thermalization coefficient;
β = sticking coefficient;

1) $\frac{d}{dt}(N_l + N_g) = 0$

mass conservation

2) $\frac{dN_l}{dt} = \beta(-\Phi_{vap} + \Phi_{cond})S_l$

vaporization condensation

3) $\frac{d}{dt}(E_l + E_g) = -P_g \frac{dV}{dt}$

Energy conservation prescribed volume expansion

4) $\frac{dE_l}{dt} = [\beta(-(c_v T_l - a n_{gas}(T_l))\Phi_{vap} + (c_v T_g - a n_g)\Phi_{cond}) + (1-\beta)\alpha\Phi_{cond} c_v (T_g - T_l)]S_l$

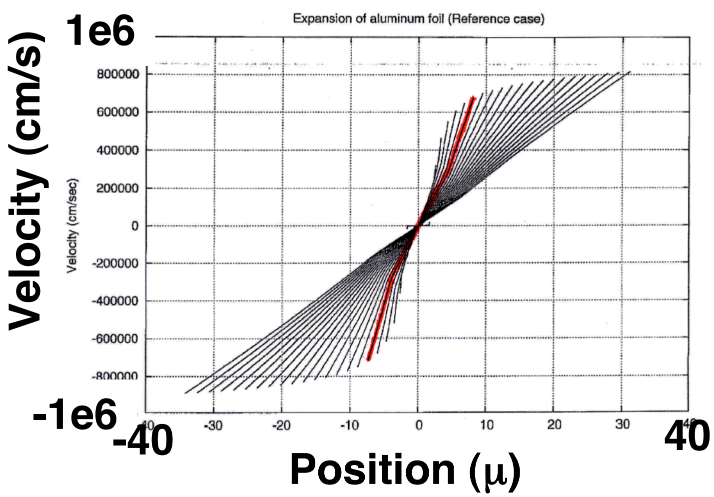
vaporization condensation thermalization by non-sticking particles

Energy of evaporating particle

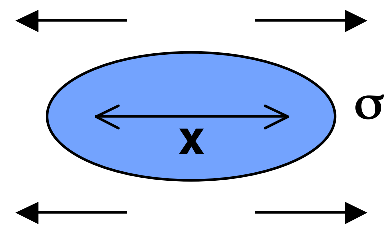
Energy of condensing particle

from Armijo and Barnard, 2007, in prep.

Characteristic size of a droplet in a diverging flow



Locally, dv/dx = const (Hubble flow)



Steady-state droplet

Equilibrium between disruptive dynamic pressure and restoring surface tension: Weber number We= inertial/surface ~ $(\rho\, v^2\, A)/\sigma\, x \sim \rho\, (dv/dx)^2\, x^4 / \sigma\, x$ ~ 1

→ <u>Characteristic size :</u>

$$\boxed{x = (\sigma / \rho\, (dv/dx)^2)^{1/3}}$$

→ Estimate : x ~ 0.05 μm

Ref: J. Armijo, master's internship report, ENS, Paris, 2006, and J. Armijo and J.J. Barnard (in preparation).

Conclusion

Hydrodynamic simulations allow predictions for WDM experiments to anticipate experimental results

Useful insight is being obtained from:

> The similarity solution found in textbooks for ideal gas equation of state and initially uniform temperature,
>
> More realistic equations of state (including phase transition from liquid, to two-phase regime)
>
> Inclusion of finite pulse duration and non-uniform energy deposition
>
> Comparisons of simulations with and without Maxwell-construction of the EOS

Work has begun on understanding the role of droplets and bubbles in the target hydrodynamics and the physics of metallic foams

References

I.D. Landau and E. M. Lifshitz, "Fluid Mechanics," [Pergamon Press, Oxford] 1959.

Ya. B. Zeldovich and Yu. P. Raizer, "Physics of Shock Waves and High-Temperature Hydrodynamic Phenomena," [Dover, New York], 1962.

F. Reif, "Fundamentals of statistical and thermal physics", [McGraw-Hill, New York], 1965.

S. I Anisimov et al, "Pulsed laser evaporation: equation of state effects," Appl Phys. A. 69, 617-620 (1999).

Sokolowski-Tinten et al, PRL 81, 224 (1998)

J. Armijo, master's internship report, ENS, Paris, (2006)

J. Armijo and J.J. Barnard (in preparation).

R. More, T. Kato, H. Yoneda, Unpublished report, National Institute for Fusion Science, Toki, Japan (2005).

R. More, H. Yoneda and H. Morikami, JQSRT 99, 409 (2006).

R. More, "Dish User Manual," LBNL Report (2007).

M. M. Marinak, G. D. Kerbel, N. A. Gentile, O. Jones, D. Munro, S. Pollaine, T. R. Dittrich, and S. W. Haan, Phys. Plasmas 8, 2275 (2001).

J.J. Barnard et al, Nucl. Inst. and Meth. in Phys. Res. A, 577, 275-283 (2007).